Sustainable Futures

Summary Assessment

Using

P2 Framework Models

This document was developed to help compile estimation results from U.S. EPA OPPT's P2 Framework Models and is used by OPPT during Sustainable Futures (SF) training described at www.epa.gov/oppt/sf.
Participants in the voluntary SF Initiative are asked to submit the information contained in this assessment along with their SF PMNs in their choice of format.

Use of this specific format is not mandatory.

Chemical Assessed:

CAS Registry Number:

Participant Name:

Date of Assessment: 23 August 2017

CAS RN: Submitter:

Record ID:	**CAS No.**
Chemical Structure	**MW:**
	MF:
	Physical Form: Liquid (aqueous solution)
	Submitter:
	Trade Name:
	Use: paint binder
	Production Volume: 1st year: 3rd year:
Is this a representative structure? Yes; the PMN substance is a mixture that meets the OECD definition of a polymer	

SMILES: Monomer =

See EPISuite outputs for additional SMILES structures:

Dimer
Trimer
Tetramer
Pentamer

Name:

Synonyms:

SUSTAINABLE FUTURES SUMMARY:

Concern Level	HIGH	MODERATE	LOW
Persistence	X		
Bioconcentration			X
Cancer Health Hazard			X
Non-Cancer Health Hazard		X	
Aquatic Toxicity Hazard		X	
Is the chemical predicted to be a PBT by PBT Profiler?	No		
Overall Hazard Concern	**Human Health Hazard:** Moderate **Aquatic Hazard:** Moderate		
Overall Risk	**Human Health Risk:** Low **Aquatic Risk:** Low		

CAS RN: Submitter:

PHYSICAL/CHEMICAL PROPERTIES: See EPISuite attachments	
Melting Point (deg C)	101 deg C (monomer); higher for oligomers
Boiling Point (deg C)	327 deg C (monomer); higher for oligomers
Boiling Point Pressure (mm Hg)	
Vapor Pressure (mm Hg)	0.000285 Pa (monomer); lower for oligomers
Water Solubility at 25 deg C (g/L)	1000 (monomer); lower for oligomers
Log K_{ow}	-1.41 (monomer) to 2.64 (pentamer)
ENVIRONMENTAL TRANSPORT AND FATE: (all properties predicted using EPISuite, unless otherwise indicated)	
Transport	
Henry's Law Constant – HLC (atm-m^3/mol)	6.28E-016 atm-m3/mole (monomer)
Soil Adsorption Coefficient – log K_{oc}	Koc = 398 (monomer)
Log Bioconcentration Factor – BCF	0.5 (monomer)
Persistence	
Probability of Rapid Biodegradation	No (monomer, slower degradation for oligomers)
Ultimate Biodeg Model	Weeks (monomer, slower degradation for oligomers)
Primary Biodeg Model	Days-Weeks (monomer, slower degradation for oligomers)
Ready Biodegradability (MITI Model)	BIOWIN5: Does Not Biodegrade Fast (monomer) Read-across: Not readily biodegradable based on analog (OECD 301B)
Atmospheric Half-life	1.02 Hrs
Hydrolysis Half-life	Not hydrolysable (monomer)
Volatilization Half-life for Model River	5.19E+10 days
Volatilization Half-life for Model Lake	5.66E+11 days
Removal in STP (EPA Draft Method)	1.85% (monomer) to 3.56% for pentamer
Experimental Data	none
Byproducts	
Degradation Products	
Metabolites	

CAS RN: Submitter:

ECOTOXICITY:	
ECOSAR Class	Aliphatic amines
Acute Toxicity	
Fish LC50	Read-across: LC50 = 3.7 mg/L by analogy to
Daphnid LC50	Read-across: LC50 = 34 mg/L, by analogy to
Green Algae EC50	Read-across: 72-h ErC50 = 44 ug/L by analogy to
Chronic Toxicity	
Fish ChV	ECOSAR Not reliable; Read-across: 0.37 mg/L derived from LC50 for analog by applying ACR of 10
Daphnid ChV	ECOSAR Not reliable; Read-across: 3.4 mg/L derived from LC50 for analog by applying ACR of 10
Green Algae ChV	Read-across: 11 ug/L (for analog derived from acute ErC50 by applying ACR of 4
Hazard Concern for Aquatic Toxicity	Growth reduction for algae
Concern Concentration	Acute CoC Fish = 0.74 mg/L (LC50/5) Daphnia = 6.8 mg/L (LC50/5) Algae = 11 ug/L (ErC50/4) Chronic CoC Fish = 37 ug/L (ChV/10) Daphnia = 0.34 mg/ L (ChV/10) Algae = 1.1 ug/L (ChV/10) **Lowest acute CoC = 11 ug/L for algae** **Lowest chronic CoC = 1.1 ug/L for algae** **(moderate concern level)** **by analogy to**
CANCER HEALTH EFFECTS:	
Experimental data	
OncoLogic Results	Low concern for silanols Low concern for aliphatic amines
Overall Hazard Concern for Carcinogenicity	Low
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Moderate by analogy to
Irritation	Positive; by analogy to

CAS RN: Submitter:

Skin Sensitizer	Positive; by analogy to
Reproductive Effects	Moderate; by analogy to NOAEL = 500 mg/kg-bw/d (highest dose tested)
Developmental Effects	Moderate; by analogy to NOAEL = 500 mg/kg-bw/d (highest dose tested)
Immune System Effects	No relevant data identified
Neurotoxicity	No relevant data identified
Genotoxicity	Low, by analogy to
Mutagenicity	Low, by analogy to
Systemic Effects	Moderate; by analogy to
Overall Hazard Concern for Non-Cancer Health Effects	Moderate

EXPOSURE MODELS:			
INDUSTRIAL RELEASE AND EXPOSURE VALUES: CHEMSTEER			
Process	manufacturing	**Number of Release Days**	23
SIC Code / NPDES #		**Number of Facilities**	1
Occupational Exposure Values			
	Cancer LADD	**Chronic ADD**	**Acute APDR**
Dermal		3.43E-04 mg/kg-bw/d	6.43E-03 mg/kg-bw/d
Inhalation		n/a	n/a
Environmental Release Values			
Release to Water [Equipment cleaning]		None - equipment cleanout waste is incinerated	
Release to Air (Fugitive) [Equipment cleaning]		None - the PMN chemical has low vapour pressure	
Release to Air (Fugitive) [loading liquid product into drums]		n/a	
Release to Landfill		n/a	
Release from Incineration		kg/site/year assuming 99% removal efficiency by incineration (based on kg/site/year releases from manufacturing and processing that are sent to incineration)	
Other Release Activities			
GENERAL POPULATION EXPOSURE VALUES: E-FAST			
Aquatic Exposure: none anticipated			
Lowest Acute COC – Aquatic Exposure		Acute CoC = 11 ug/L (by analogy to	
Lowest Chronic COC – Aquatic Exposure		Chronic CoC = 1.1 ug/L (by analogy to)	
Predicted Environmental Concentration (PEC)		No releases to water from manufacture or processing PEC from use (water) < 0.01 parts per trillion	
PEC Exceeds Chronic COC (days / year)		0 (zero)	
Human Exposure: all PMN substance wastes from MFR, PROC incinerated			
	Cancer LADDpot	**Chronic ADDpot**	**Acute ADRpot**

CAS RN: Submitter:

Drinking Water			
Fish Ingestion			
Fugitive Emissions [drumming]			
Fugitive Emissions [reactor cleaning]			
Incineration Emissions	kg/yr all sites		
Landfill Leaching			
Dermal – Consumer Use			
Inhalation – Consumer Use			

RISK ASSESSMENT CALCULATIONS:	
MOE – Acute Occupational Exposure	
MOE – Chronic Occupational Exposure	
MOE – Acute General Population Exposure	No general population exposure
MOE – Chronic General Population Exposure	No general population exposure

CAS RN: Submitter:

Aquatic Hazard

Acute aquatic toxicity values have been measured for algae, daphnia, and fish. NOECs were 18 ug/L, 18 mg/L and 0.63 mg/L respectively. The chronic concentration of concern, CoC was derived from the acute NOEC using the acute-to-chronic ratio and an additional assessment factor of 10 for the algae data (lowest NOEC). A chronic endpoint value between 0.1 and 10 mg/L indicates a moderate level of concern for aquatic toxicity.

Human Health Cancer Hazard

No data were identified for the PMN substance or its analogues that indicate a concern for carcinogenicity. Overall there appears to be a low concern for carcinogenicity for the PMN substance based on several factors:
1) no structural alerts
2) lack of classification by Oncologic
3) Analogues were negative in tests for genetox and mutation assays.

Human Health Non-Cancer Hazard

Acute effects (eye irritation, skin sensitization) have been observed with structural analogs of the PMN substance. However, no significant effects were observed in a 28-day combined reproductive/developmental toxicity test in rats. This study therefore yielded a NOAEL of 500 mg/kg-bw/d, the highest dose tested. This suggests a low to moderate degree of concern for non-cancer health effects from the PMN substance.

Human Health Risk Assessment

Risk assessed by calculating a margin of safety (MoS) for occupational exposure for the relevant routes of exposure. The hazard values used for quantitative risk assessment were the Derived No Effect levels (DNELs) for the analogue CAS
Only a qualitative assessment for the eye irritation and skin sensitization endpoints was done.

Abbreviations Used

CAS RN: Submitter:

Table I - Selected Analogues

Analog	Structure	Concern Identified	Basis of Concern	Concern Level
		Severe eye irritation, corrosion Skin sensitization	Experimental data	High
		Severe eye irritation, corrosion Skin sensitization	Experimental data	High

References

CAS RN: Submitter:

Appendix 1: Determination of Aquatic Risk

Chemical Identifier: **CAS Number:**

Release Activity 1: **Site Information:**

	Endpoint	**Effect Level (ppb)**	**Assessment Factor**	**Acute COC (ppb)**	**PEC (ppb)**	**Potential for Risk?**
Acute Profile	96-h Static Acute, Rainbow Trout	LC50 = 3.7 mg/L NOEC = 0.63 mg/L	5	0.74 mg/L	< 0.01 pptr	N
	48-h Static Acute, Daphnia magna	LC50 = 34 mg/L NOEC = 18 mg/L	5	0.68 mg/L	< 0.01 pptr	N
	96-h Algae, Pseudokirchneriella subcapitata	72-h ErC50 = 44 µg/L NOECr = 18 µg/L	4	11 ug/L	< 0.01 pptr	N
Chronic Profile	**Endpoint**	**Effect Level (ppb)**	**Assessment Factor**	**Chronic COC (ppb)**	**Days/Year PEC Exceeds COC**	**Potential for Risk?**
	Fish ChV	LC50/10 = 0.37 mg/L	10	0.037 mg/L	0	N
	Daphnia ChV	LC50/10 = 0.34 mg/L	10	0.034 mg/L	0	N
	Algae ChV	LC50/10 = 4.4 ug/L	10	0.44 ug/L	0	N

CAS RN: Submitter:

Appendix 2: Determination of Human Health Risk from Occupational Exposure

Chemical Identifier: **CAS Number:**

Exposure Activity 1: **Site Information:**

	Endpoint (Concern Effect)	**NOAEL (mg/kg-d)**	**LOAEL (mg/kg-d)**	**Exposure Dose and Source (mg/kg-d)**	**MOE***	**Potential for Risk?**
Occupational Exposure	Systemic toxicity	500 mg/kg-bw/d	n/a	1 mg/kg-bw/d (with PPE)	500	No

CAS RN: Submitter:

Appendix 3: Determination of Human Health Risk to the General Population and Consumers

Chemical Identifier: **CAS Number:**

Exposure Activity 1: **Site Information:**

	Endpoint (Concern Effect)	**NOAEL (mg/kg-d)**	**LOAEL (mg/kg-d)**	**Exposure Dose and Source (mg/kg-d)**	**MOE***	**Potential for Risk?**
General Population Exposure	n/a					
Consumer Exposure	n/a					